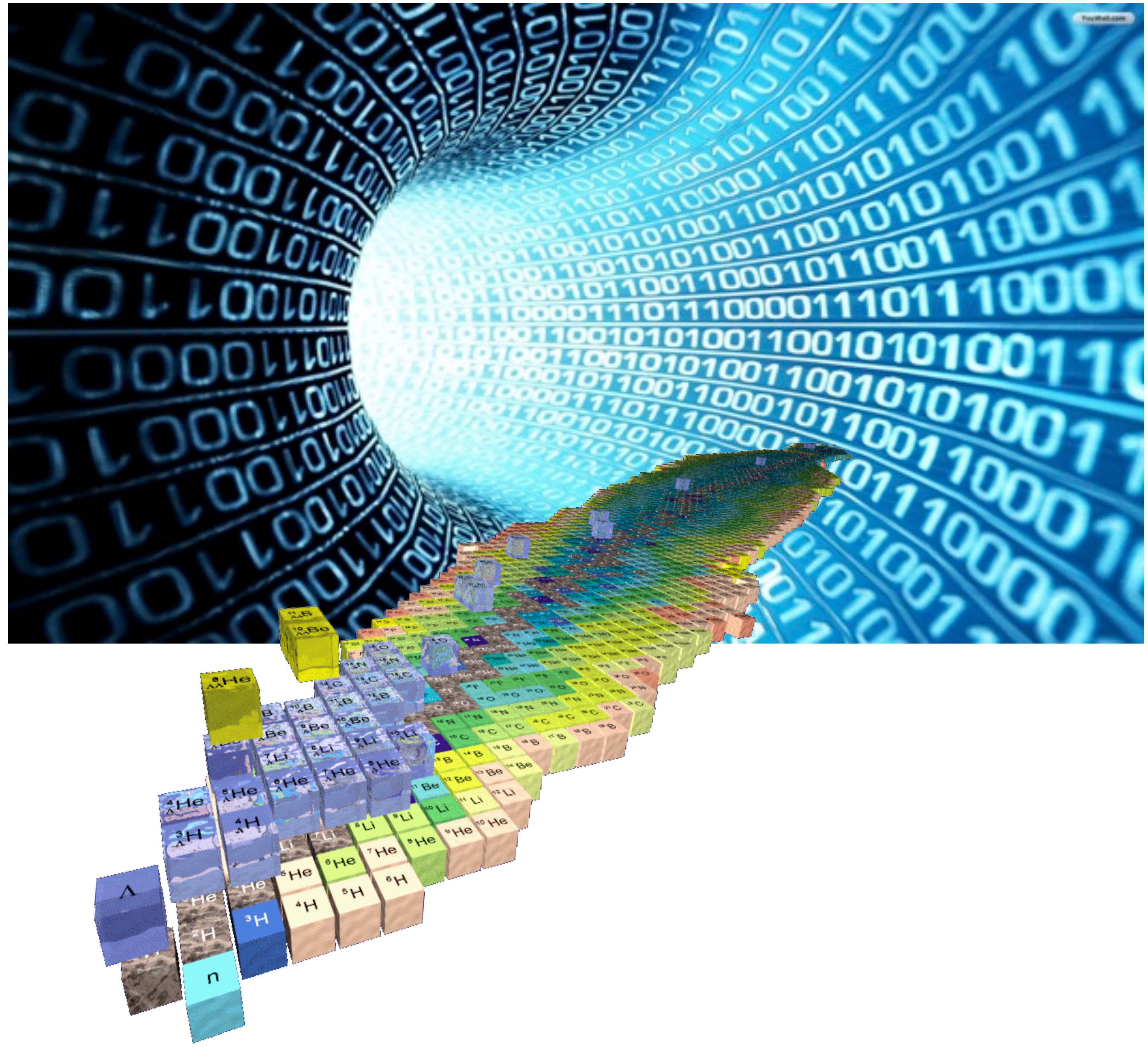
INSTITUTE for NUCLEAR THEORY

NPLQCD

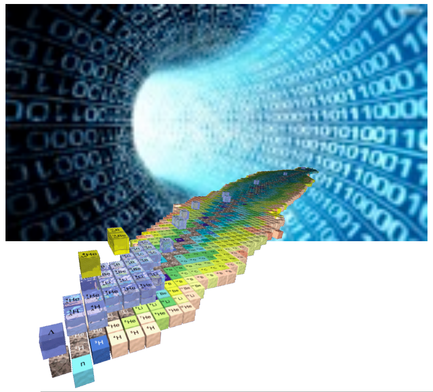


Nuclear Forces from Lattice Quantum Chromodynamics

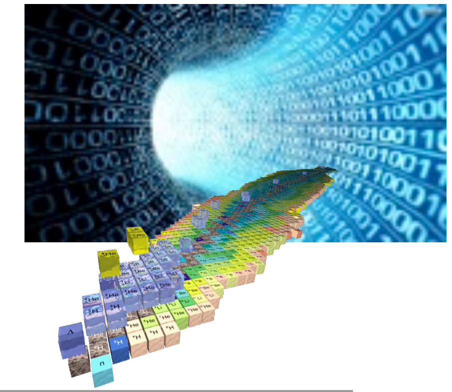
Martin J. Savage
Institute for Nuclear Theory

Large Scale Computing and Storage Requirements for Nuclear Physics (NP): Target 2017

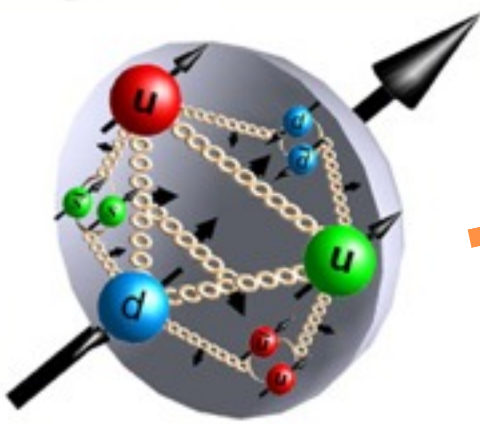
April 2014

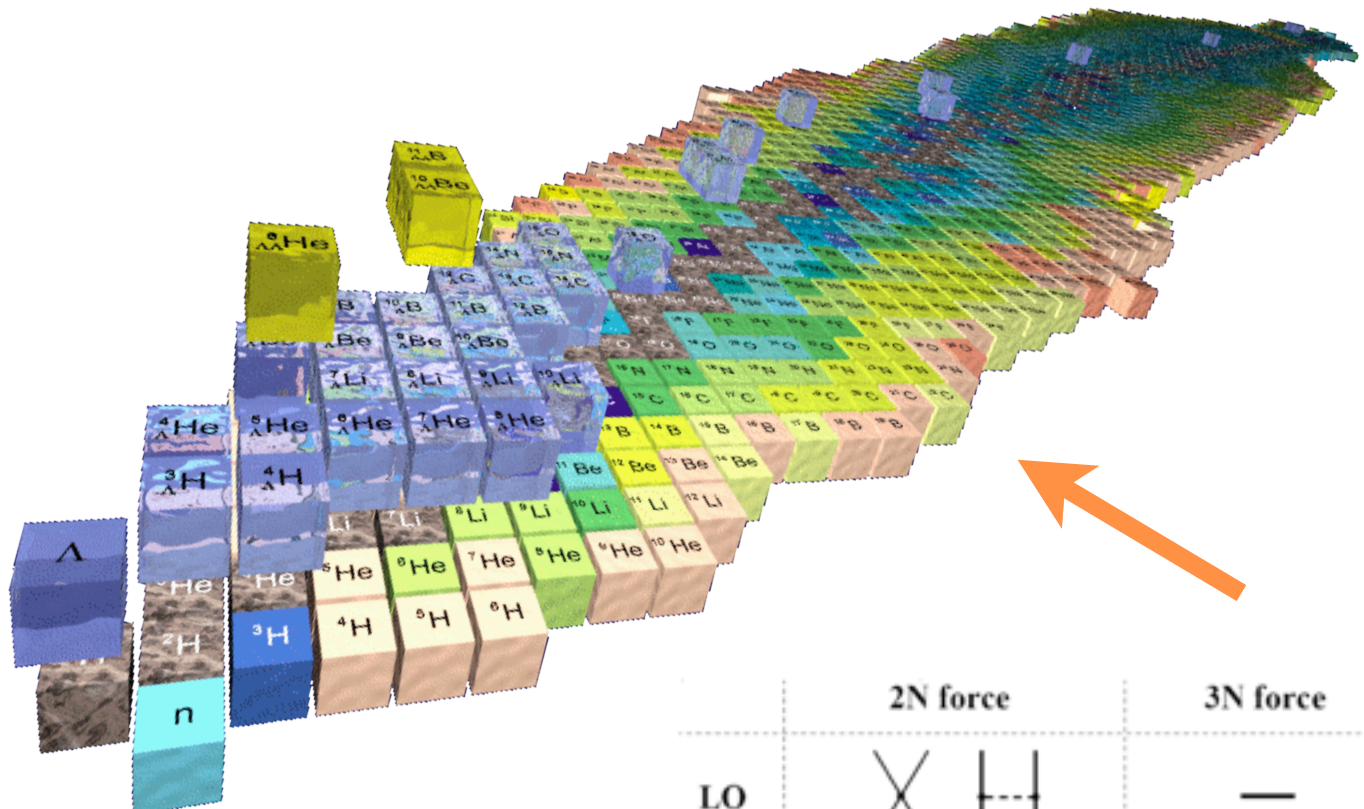


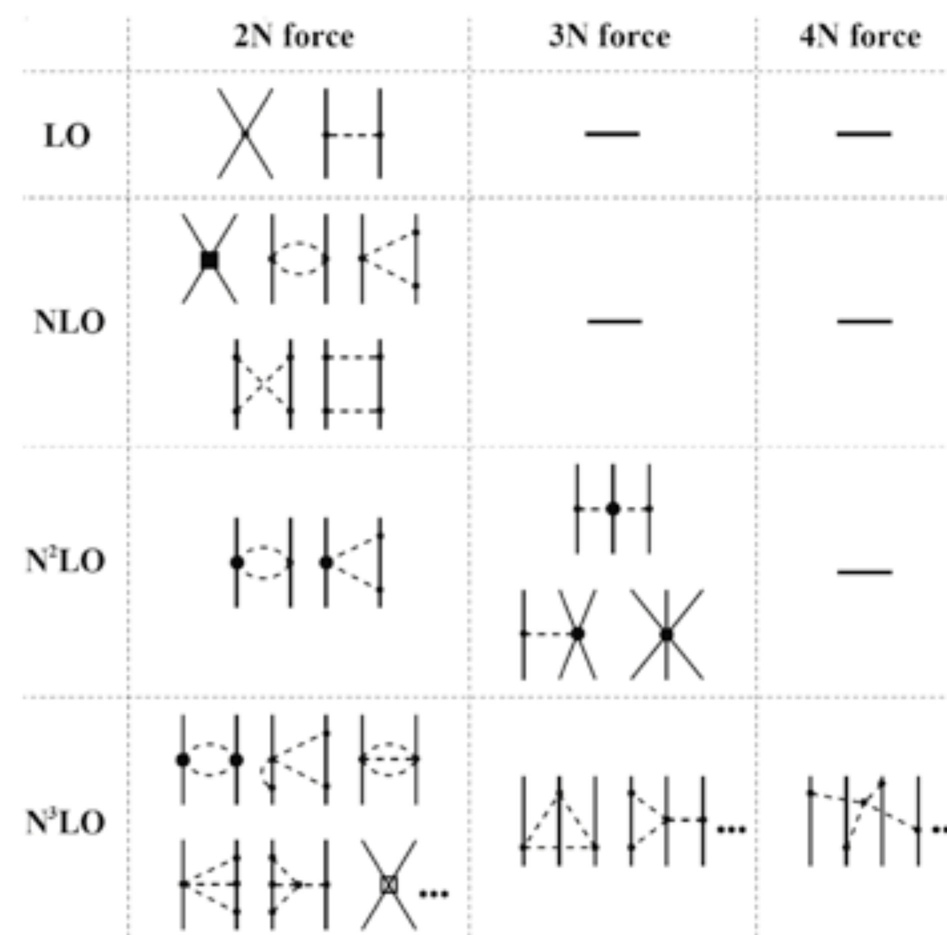
From QCD to Nuclei



FRIB



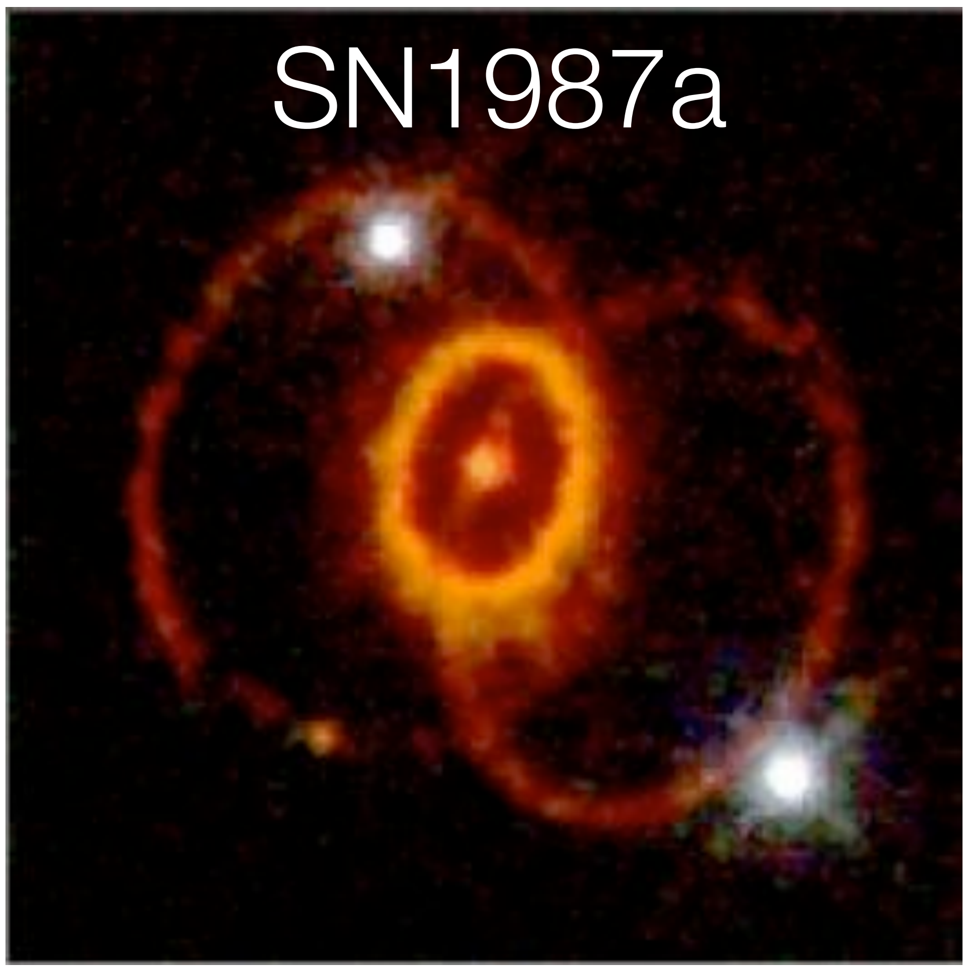




Solve QCD

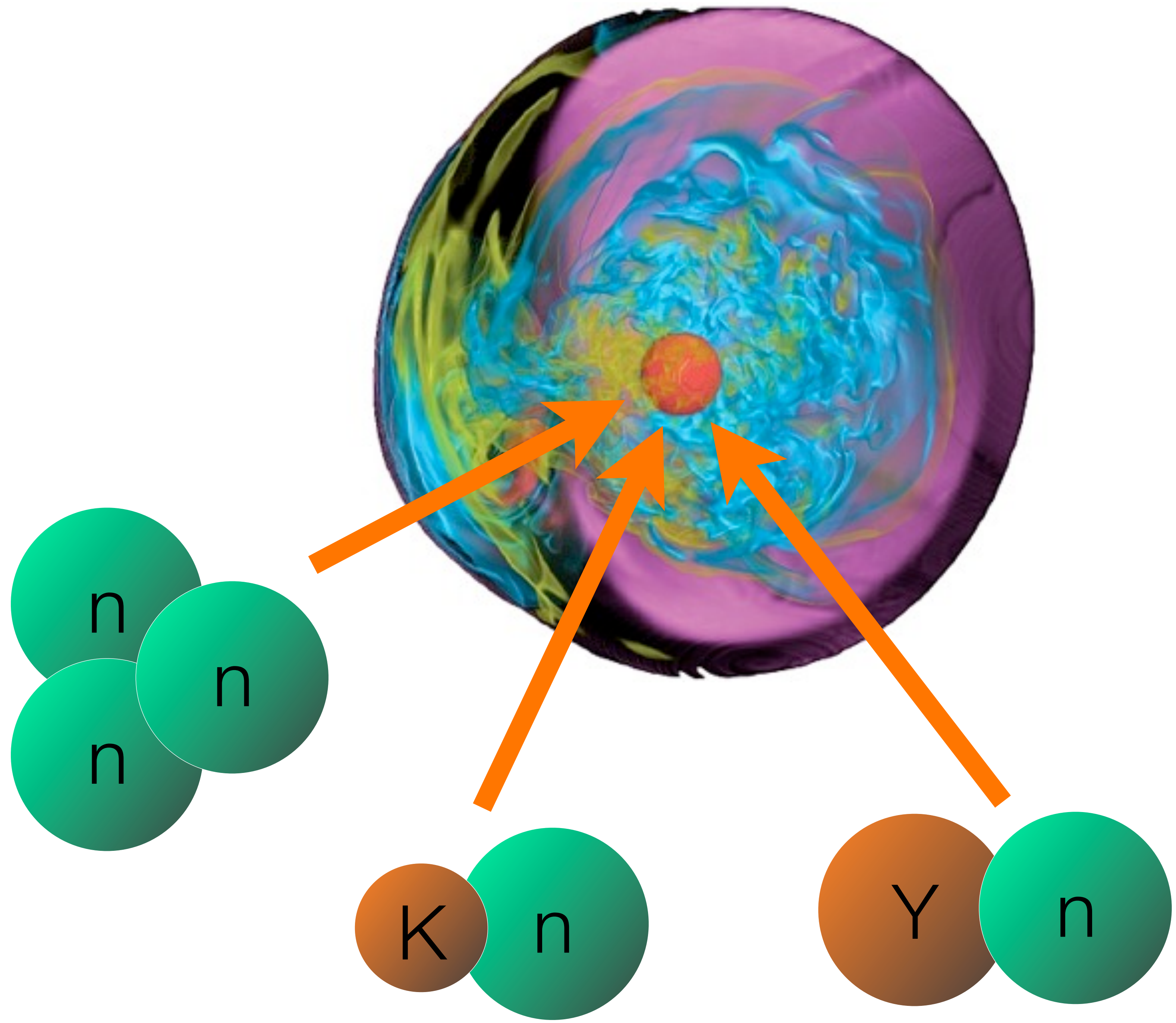
Lattice QCD

Core-Collapse Supernova

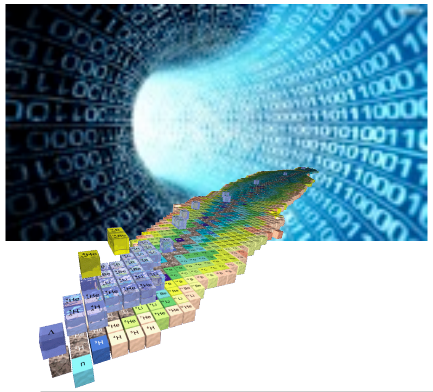


Black-Hole or
Neutron Star ?

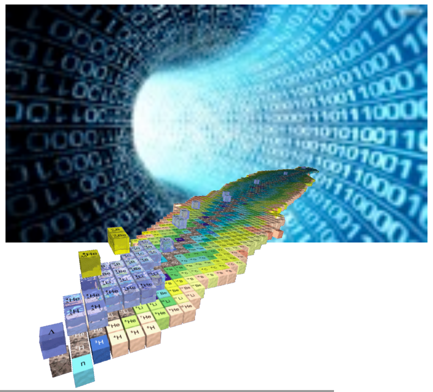
(Mezzacappa *et al*)

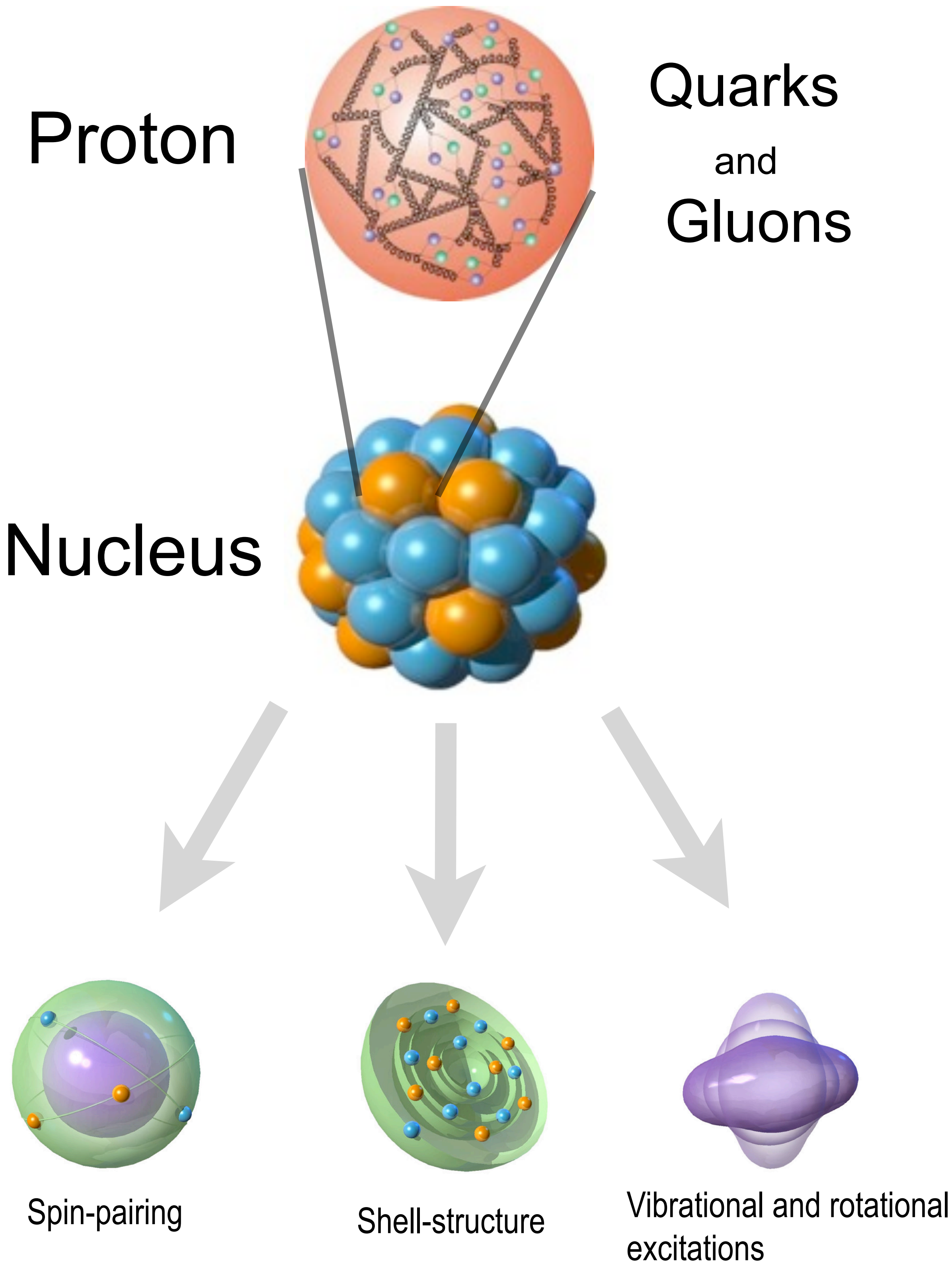


Nuclear EoS



The Structure and Interactions of Matter from QCD





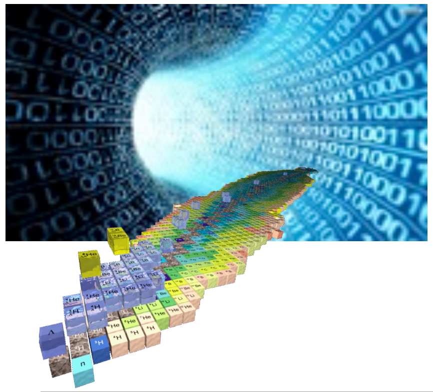
Quantum Chromodynamics

$$\Lambda_{\mathrm{QCD}}$$

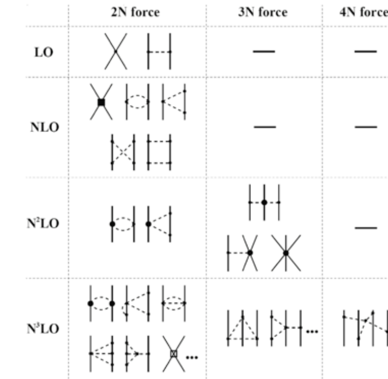
$$\frac{m_u}{\Lambda_{\mathrm{QCD}}} \qquad \frac{m_d}{\Lambda_{\mathrm{QCD}}} \qquad \frac{m_s}{\Lambda_{\mathrm{QCD}}}$$

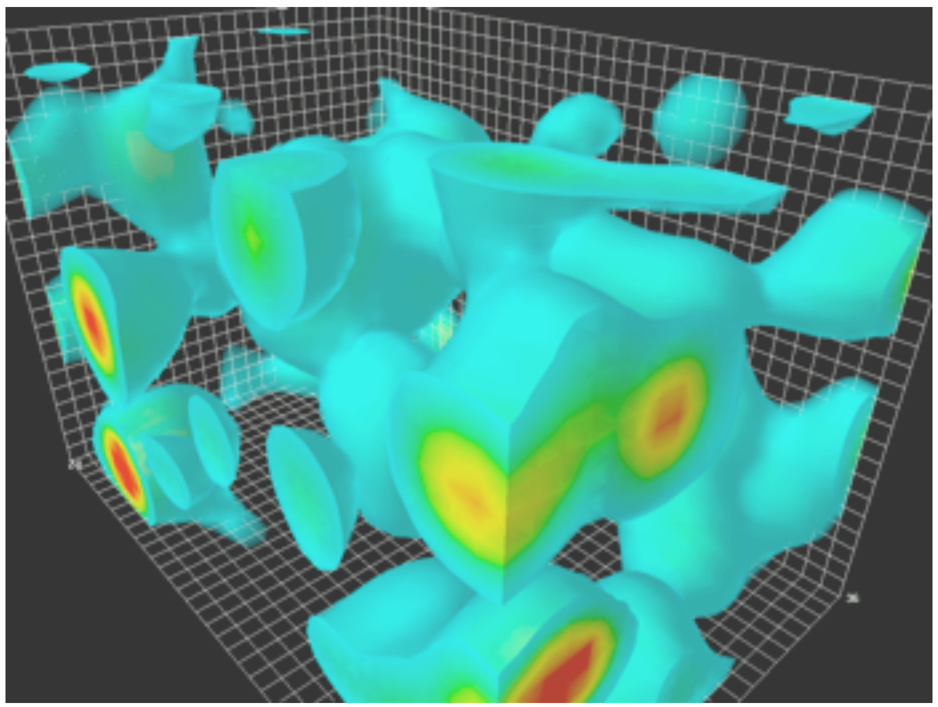
$$\alpha_e$$

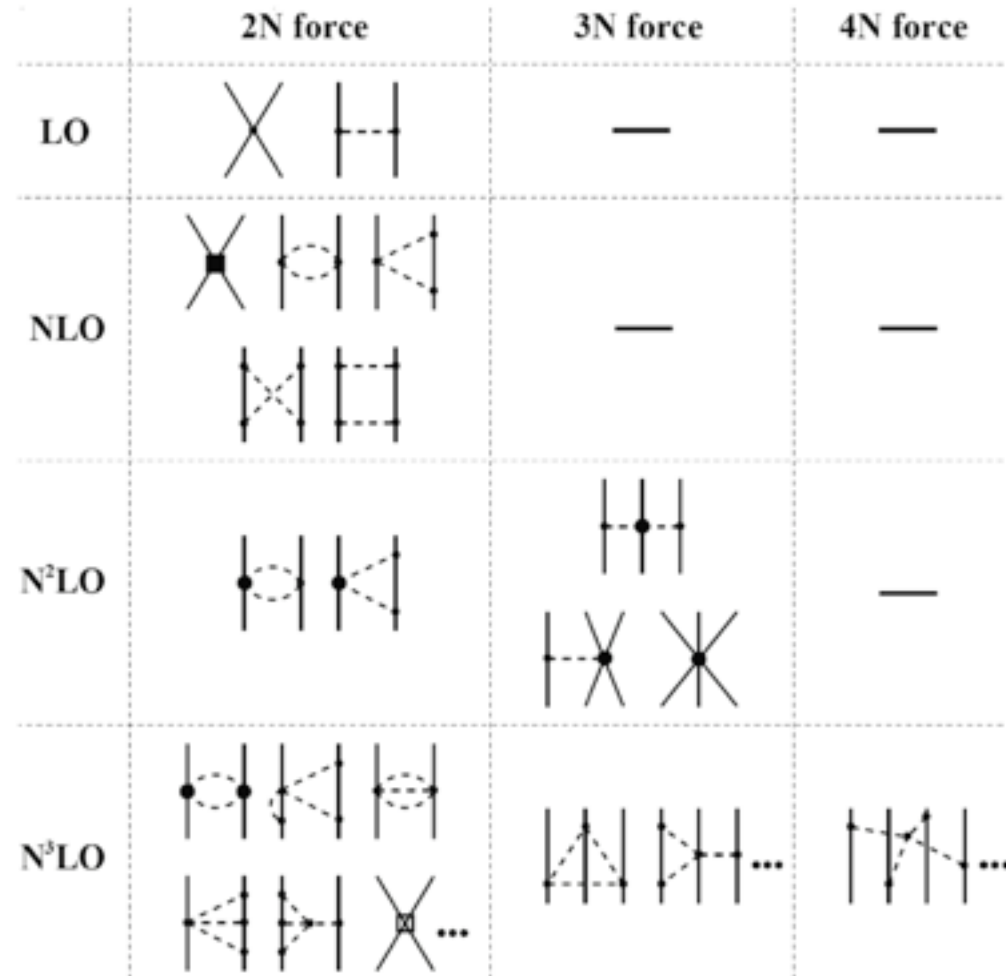
Small number of input parameters responsible for all of strongly interacting matter



Refining Nuclear Forces and Multi-Nucleon Interactions: Enhanced Predictive Capabilities







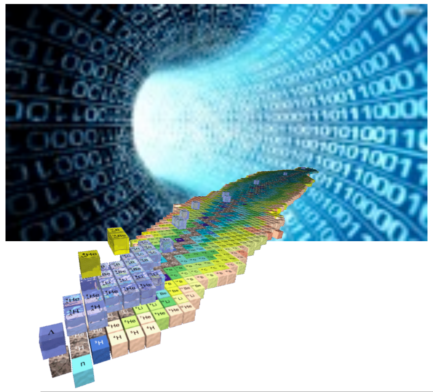
QCD to constrain coefficients

i) Verification and/or better experiment (?)

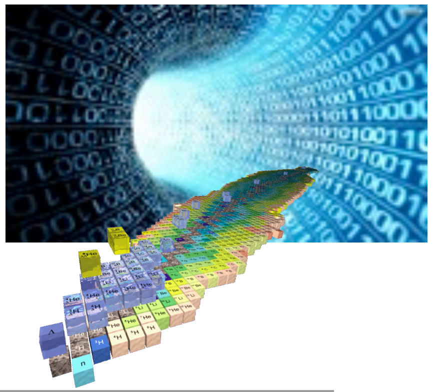
ii) Inaccessible to experiment, e.g. nnn, nnnn

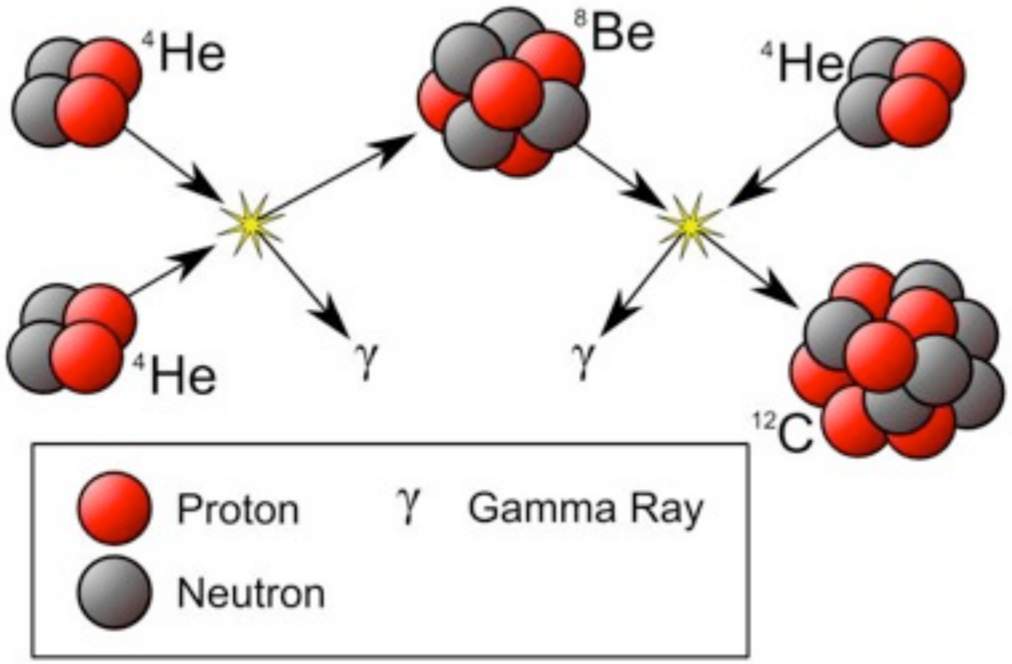
iii) Number of coefficients for required level of precision

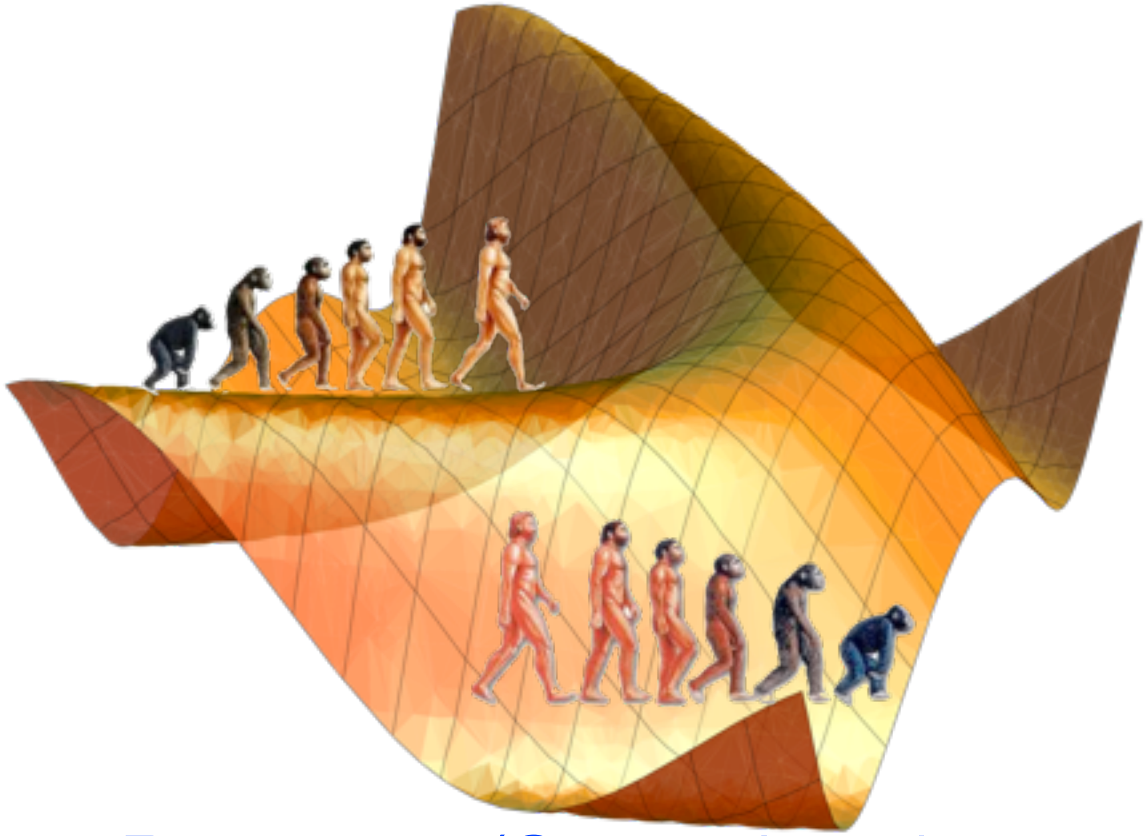
iii) and/or direct calculation of desired quantity



The ONLY way to understand Fine-Tunings of our Universe

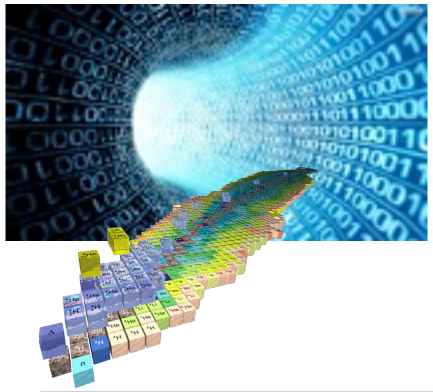






Parameter/Gauge Landscape

- Nuclear physics exhibits fine-tunings
  - *Why ??*
  - *Range of fundamantal parameters to produce sufficient carbon ?*
  - *Solving QCD is the only way to provide precise constraints.*



NSAC Milestone

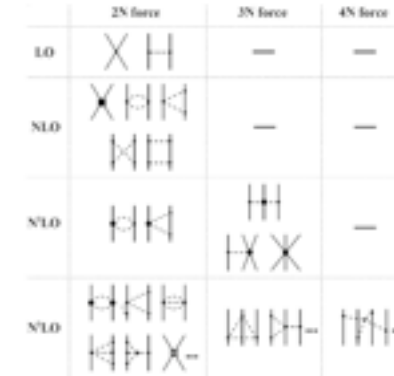


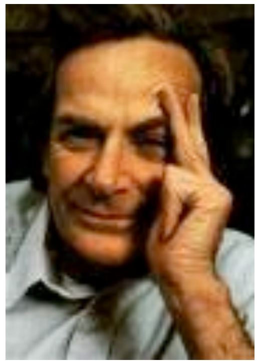
Table 4: Milestone Progress in Hadronic Physics

Year	Milestone	Complete?	Status Assessment
2014 HP10	Carry out ab initio microscopic studies of the structure and dynamics of light nuclei based on two-nucleon and many-nucleon forces and lattice QCD calculations of hadron interaction mechanisms relevant to the origin of the nucleon-nucleon interaction.	No	Expect to Achieve 2008

[assumed Moore's Law increases]

By 2017 : calculations at mpi ~ 220 MeV (140 MeV ?) will provide first direct connection to nuclear forces in nature.

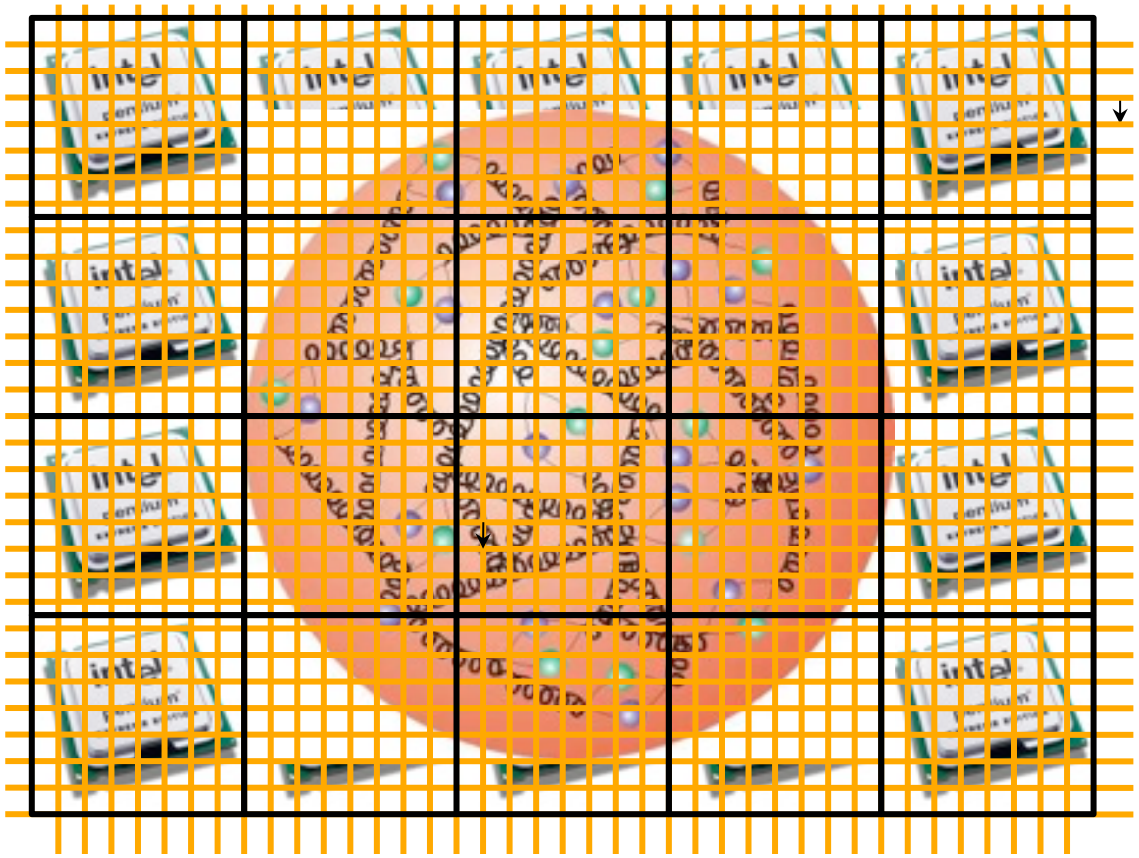
Lattice QCD



Monte-Carlo Evaluation of QCD Path Integral

Propagators Gauge Configurations

$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_\mu \; \hat{\theta}[\mathcal{U}_\mu] \; \det[\kappa[\mathcal{U}_\mu]] \; e^{-S_{YM}} \rightarrow \frac{1}{N} \sum_{\text{gluon cfgs}}^{N} \hat{\theta}\,[\mathcal{U}_\mu]$$



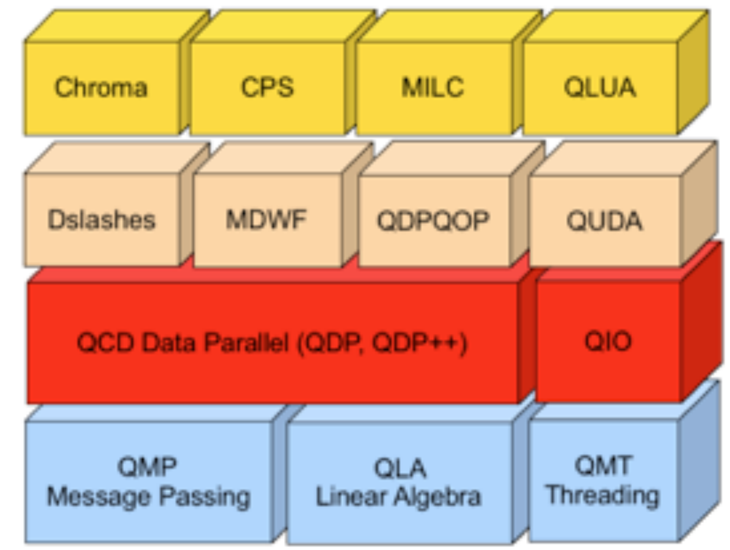
Not Quite QCD !

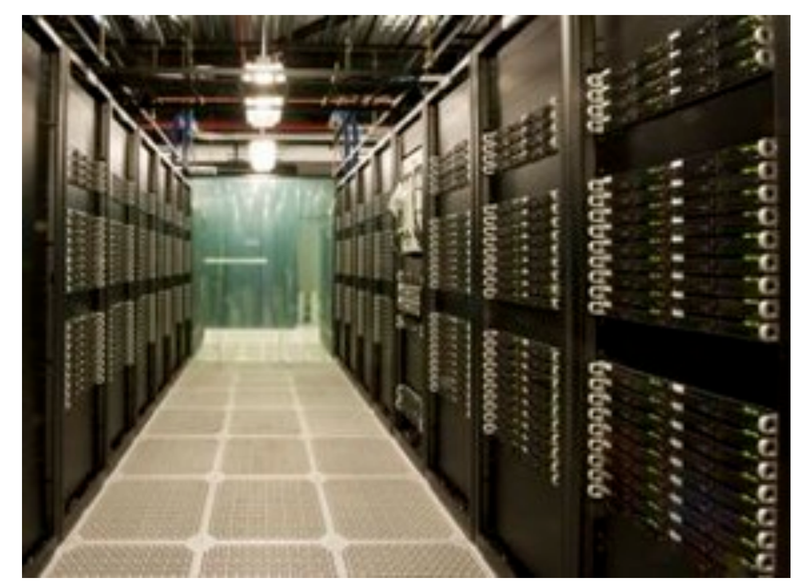
Lattice Spacing : $a << 1/\Lambda\chi$ (Nearly Continuum)

Lattice Volume : $m_\pi L >> 2\pi$ (Nearly Infinite Volume)

Systematically Extrapolate

Effective Field Theory gives form of extrapolation $a = 0$ and $L = \infty$

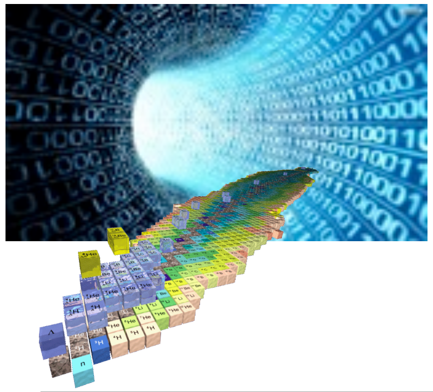




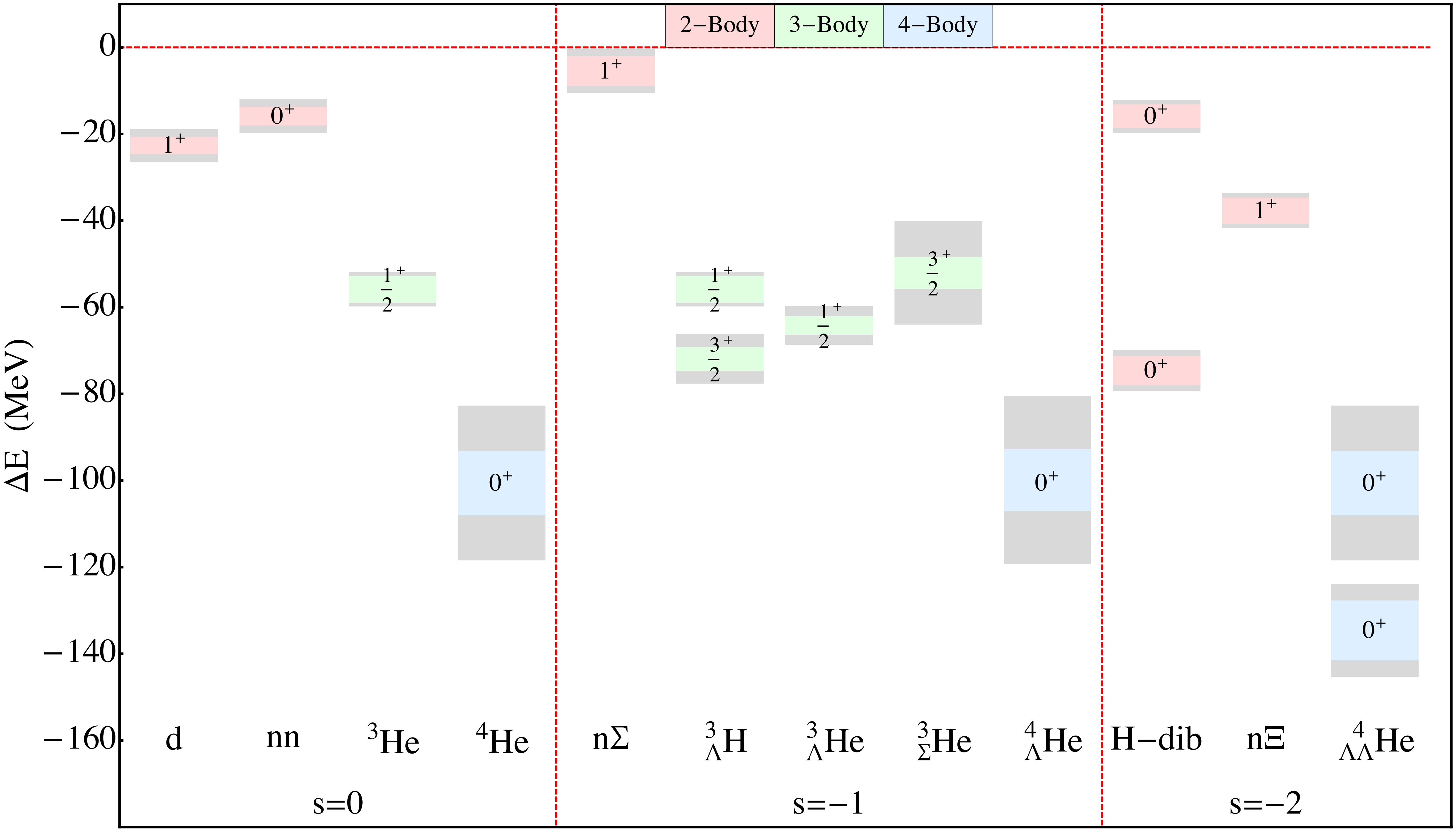
SciDAC-3 NP/HEP

capacity hardware

JLab effort is critical for NPLQCD

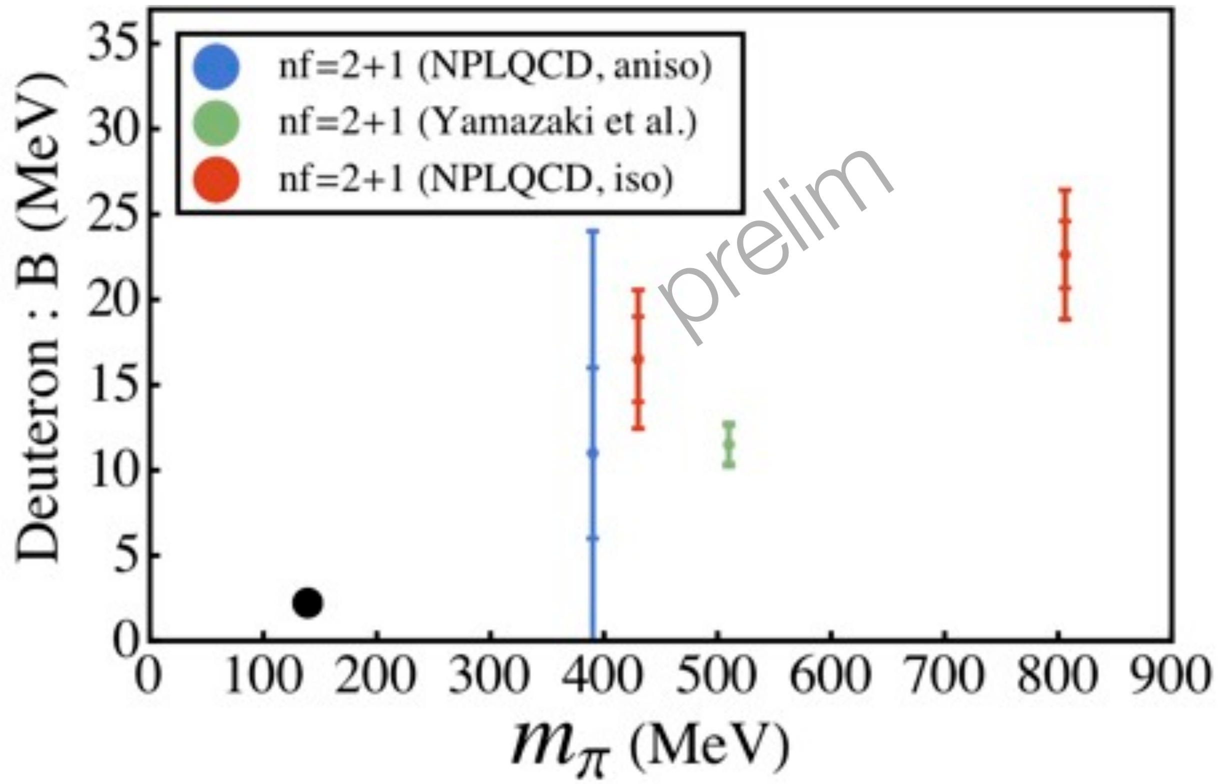


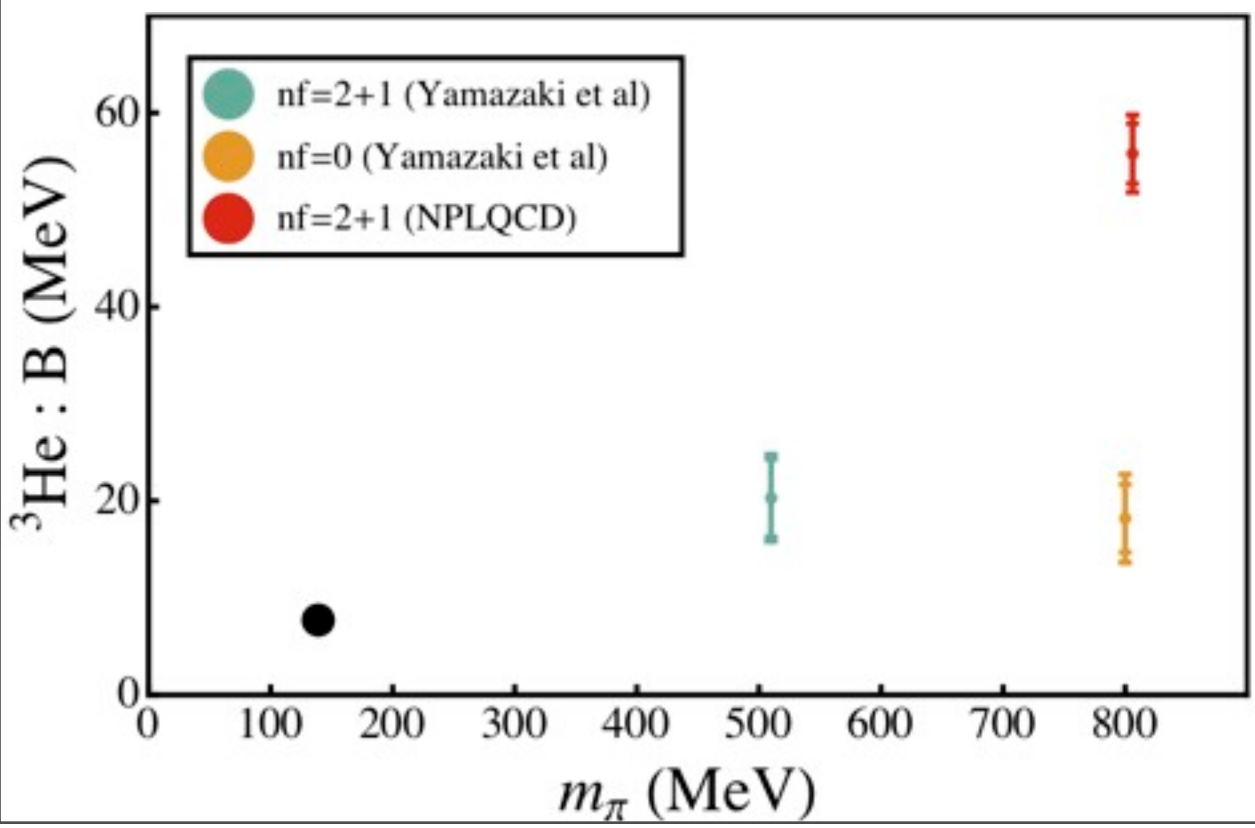
Nuclei

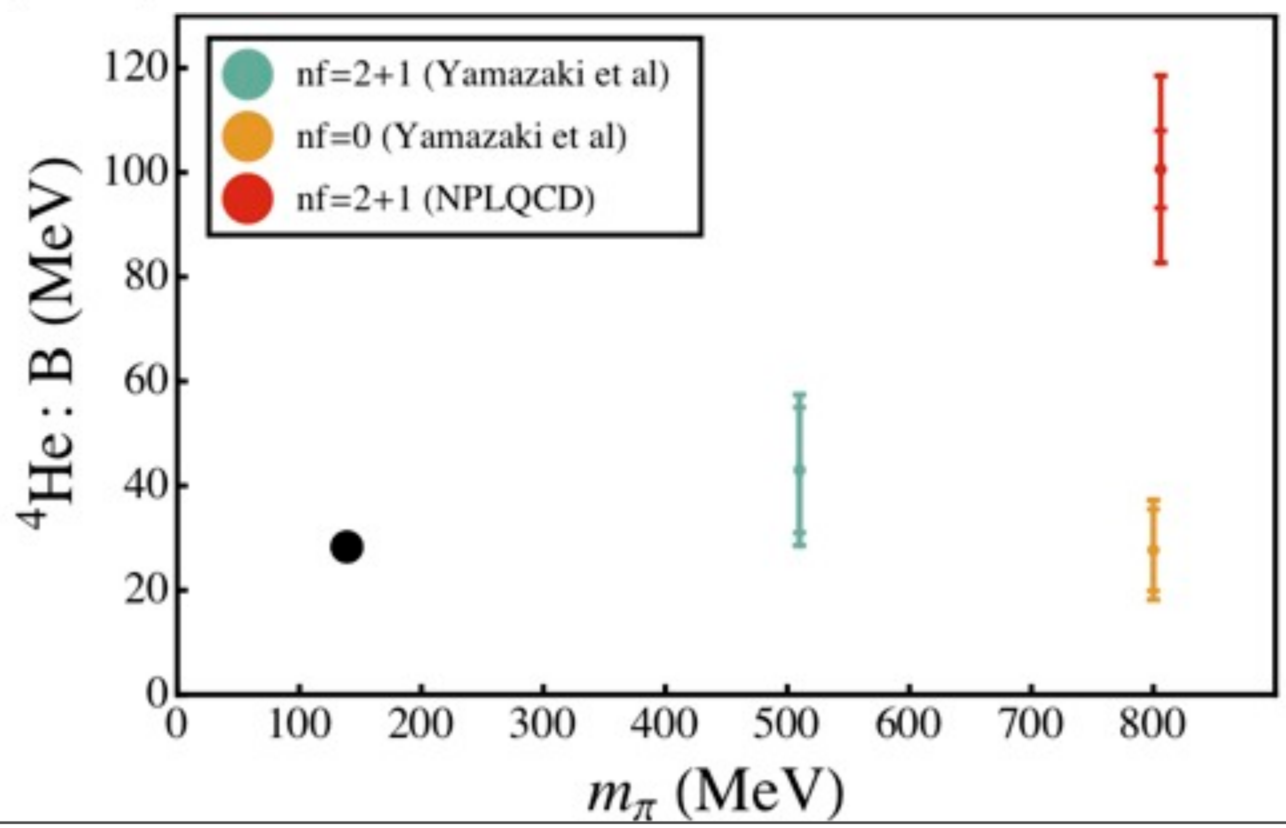


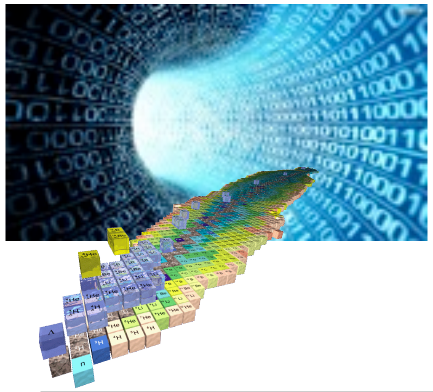
$m_\pi \sim 800$ MeV

Deuteron and Helium







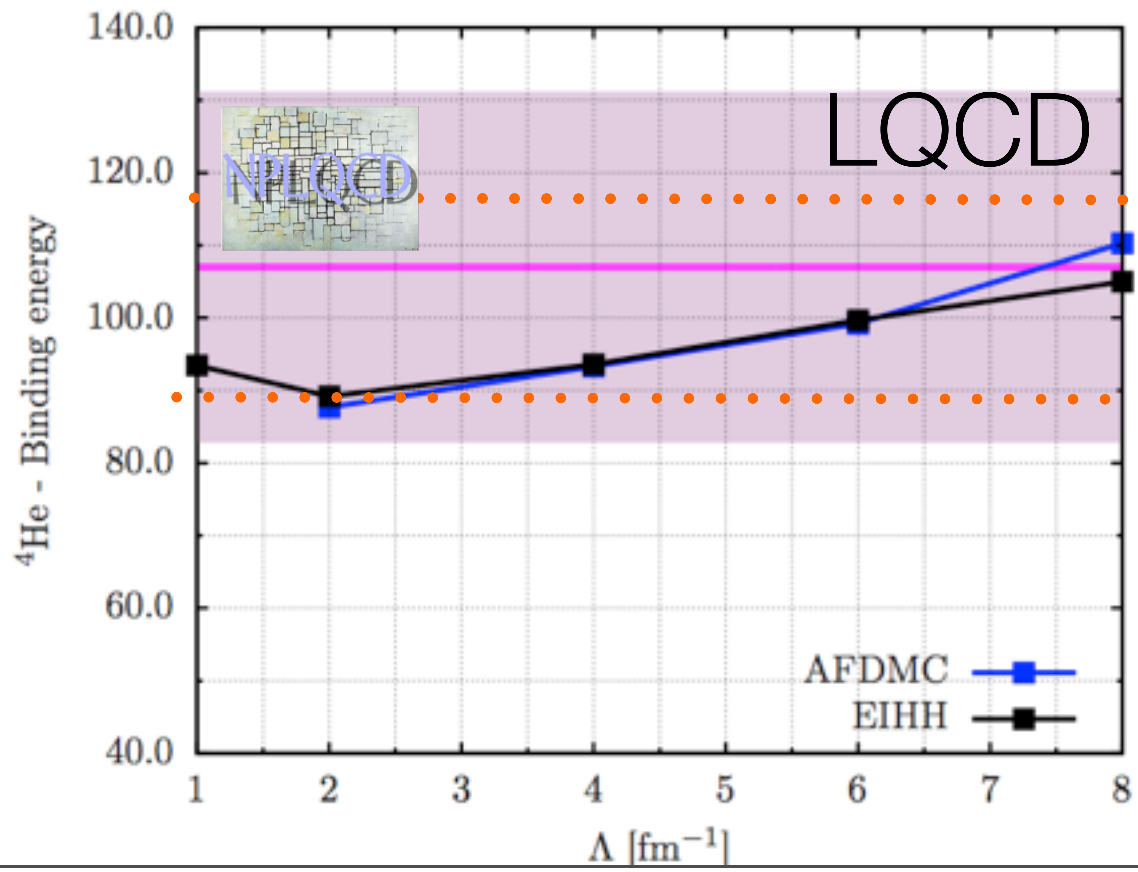


LQCD to EFT to Nuclei

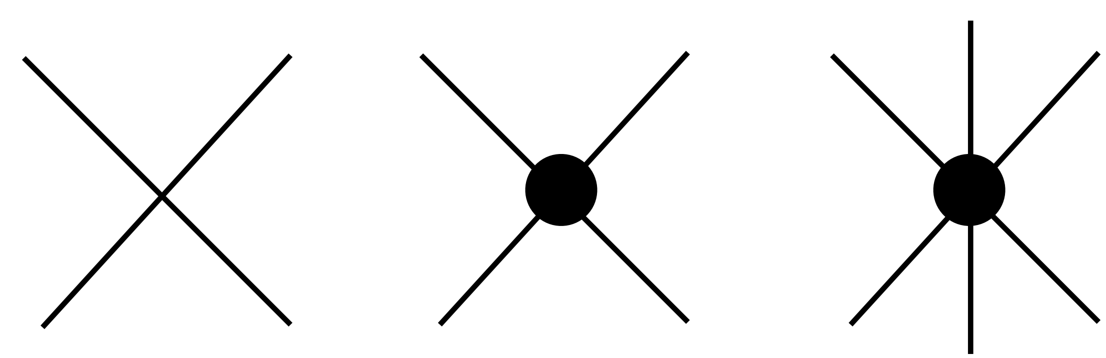
LQCD Nuclei for 800 MeV pions

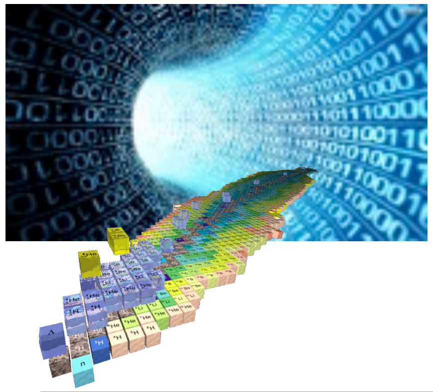
- Fit 2-body and 3-body LQCD bindings
- Predict 4-body, c/w LQCD prediction
- Predict A>>4, beyond present LQCD capabilities

Barnea, Conressi, Gazit, Pederiva and van Kolck
arXiv:1311.4966

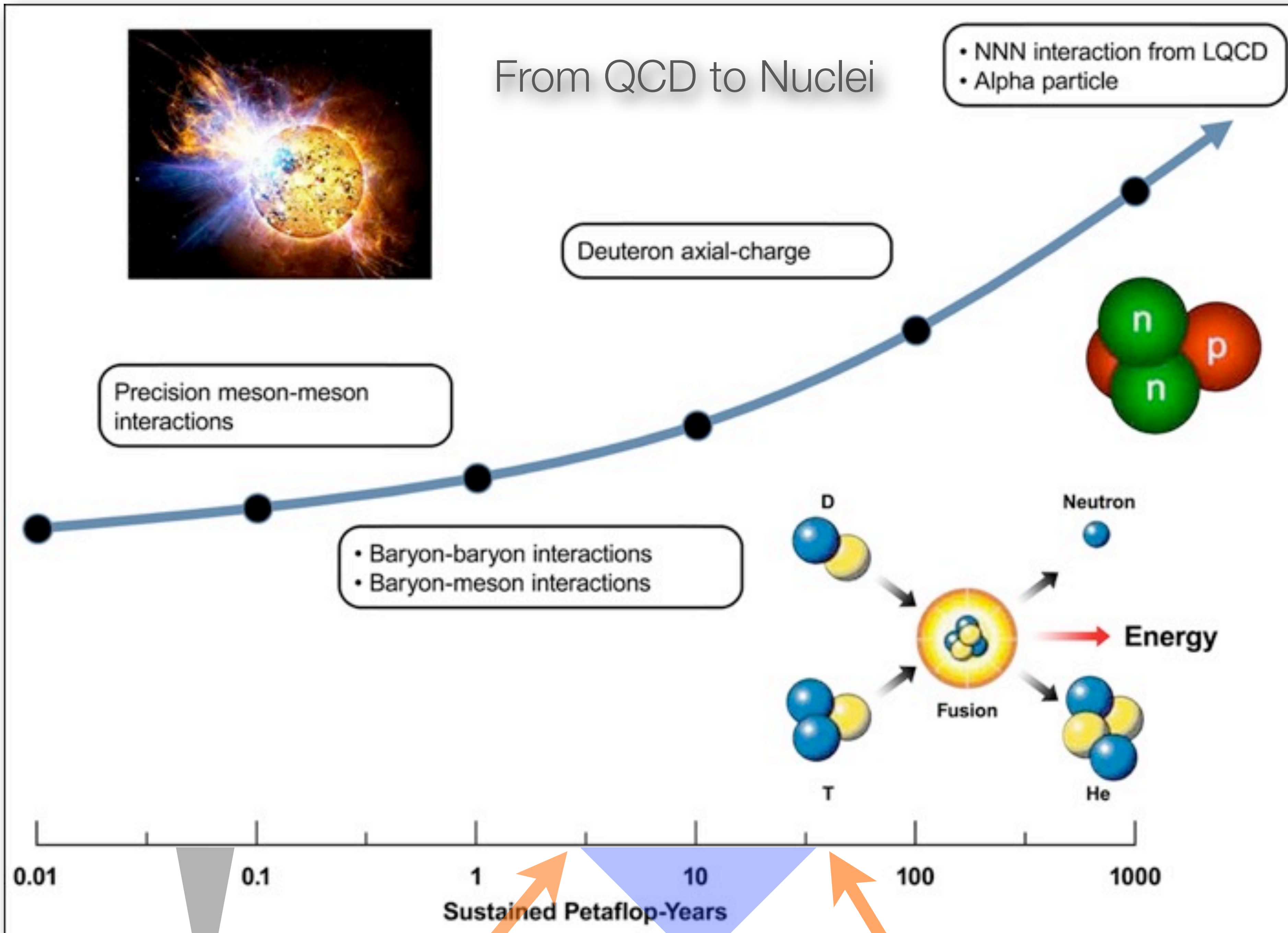


``First Contact``





Desired Resources 2014-2017

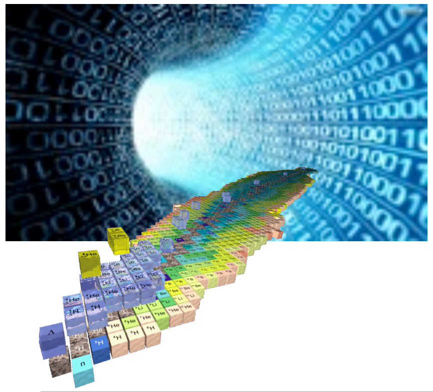


2018

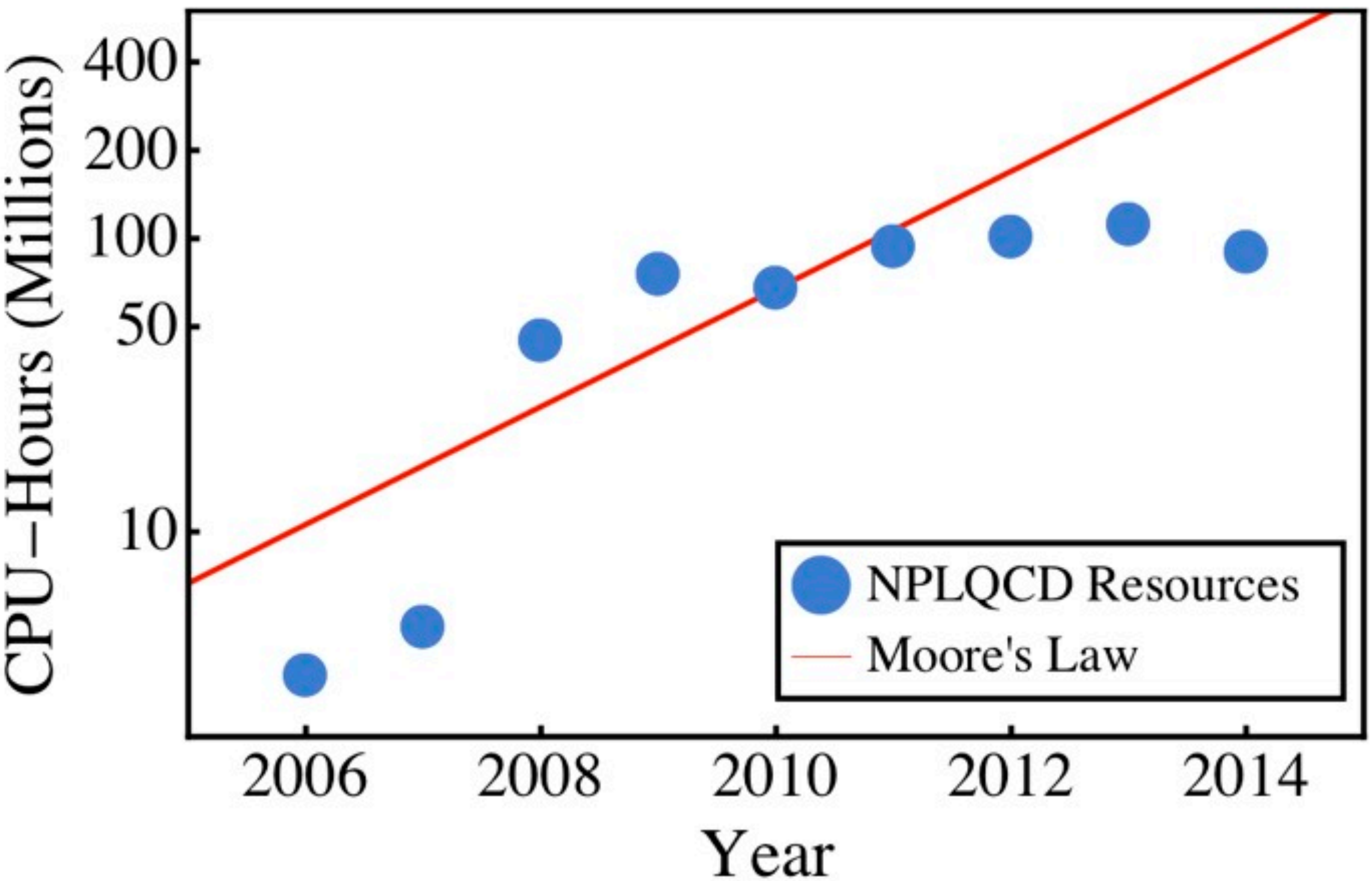
2014

Moore's Law from 2011

Moore's Law + possible Algorithm Development

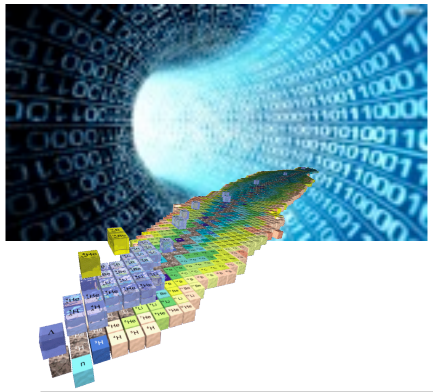


Roadblocks of the Present



> 1 year behind schedule

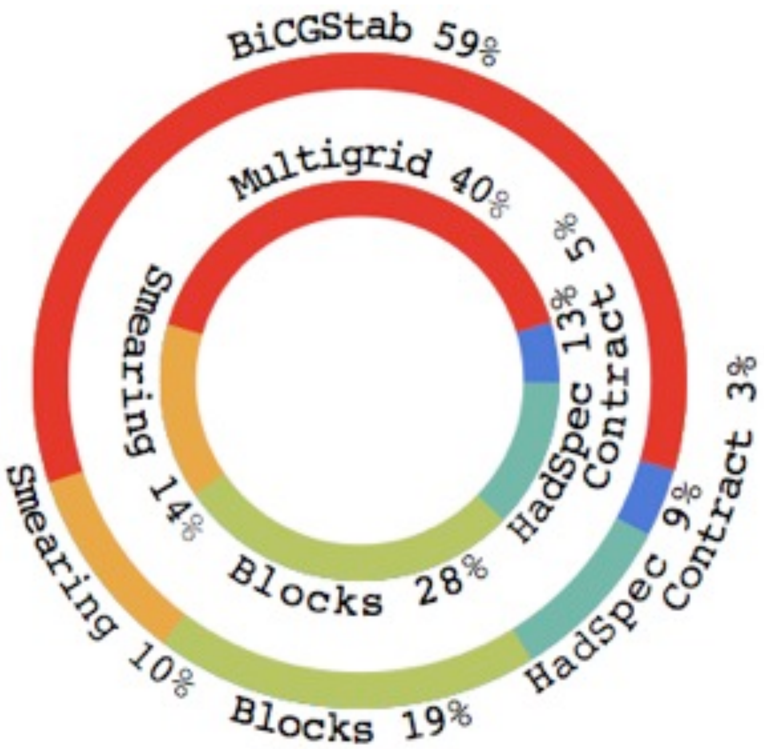
Does NOT include shared configuration production

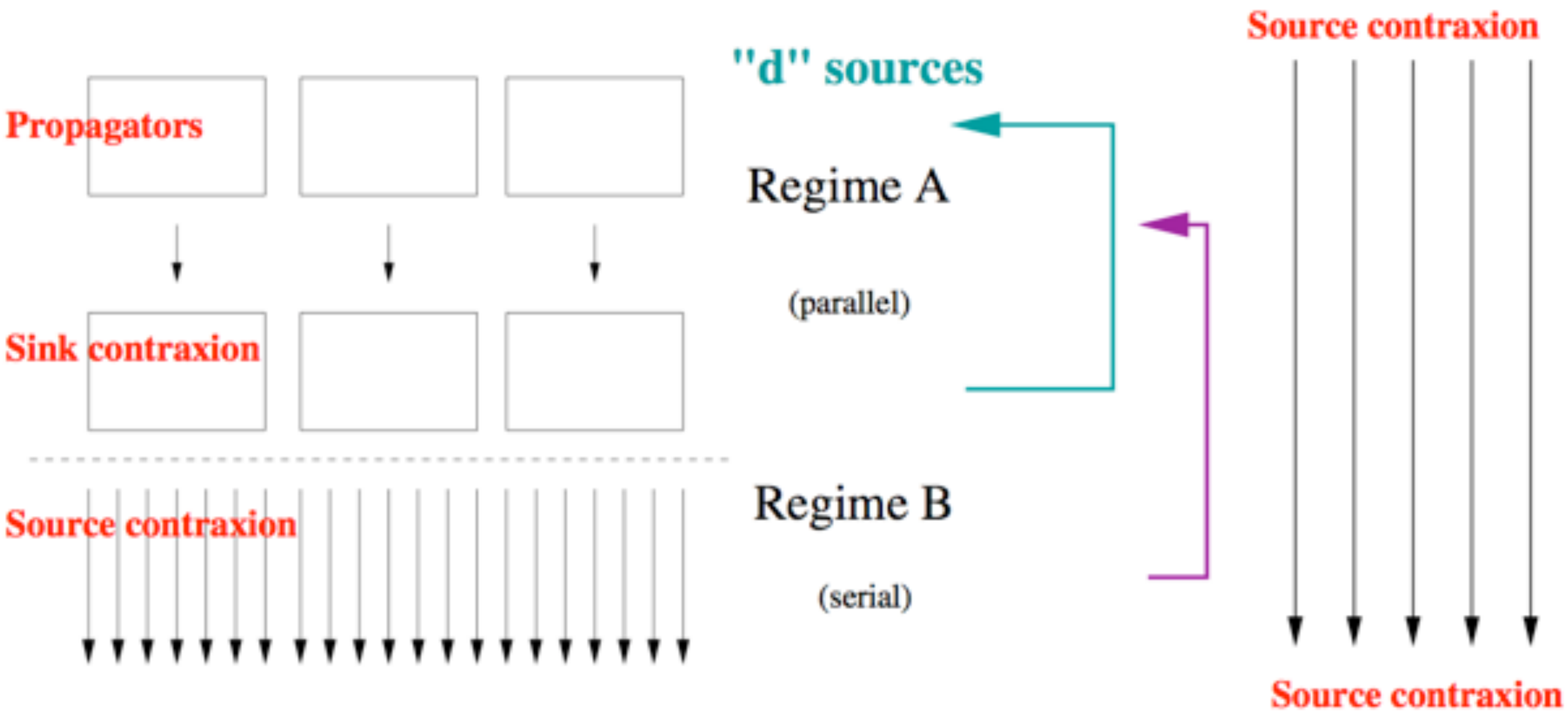


USQCD Proposed Production 2014-2019

$N_s^3 \times N_t$	Action	a fm	m_π MeV	$m_\pi L$	$m_\pi T$	Traj.	Configs. (TF-yrs)	Str-A	Str-B (TF-yrs)	HSp	HI
$64^3 \times 128$	W	0.076	250	6.1	12.3	5×10^3	8				
$64^3 \times 128$	W	0.09	200	5.8	11.7	5×10^3	9			167	27
$32^3 \times 512$	AW	0.12	200	3.8	17.6	1×10^4	44			41	
$48^3 \times 512$	AW	0.12	200	5.8	17.6	1×10^4	197			142	
$48^3 \times 192$	W	0.09	140	3.0	12.3	5×10^3	7	40			
$64^3 \times 192$	W	0.09	140	4.1	12.3	5×10^3	21	40			
$96^3 \times 64$	W	0.09	140	6.1	4.1	5×10^3	24	13			
$96^3 \times 96$	W	0.09	140	6.1	6.1	5×10^3	40	20			
$96^3 \times 192$	W	0.076	140	6.1	12.3	5×10^3	96	40	350*	334	288
$128^3 \times 192$	W	0.076	140	6.9	10.4	5×10^3	323	67		792	970
$48^3 \times 96$	DWF	0.110	140	3.9	7.8	5×10^3		28	$360^\dagger$		
$64^3 \times 128$	DWF	0.086	140	3.9	7.8	5×10^3		64	$844^\dagger$		

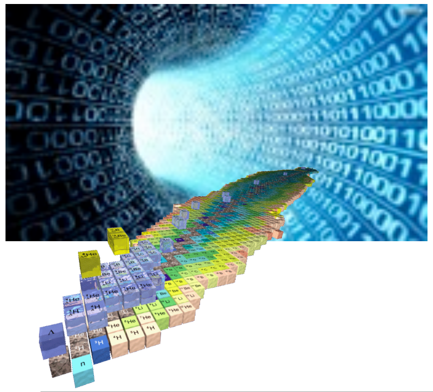
Workflow



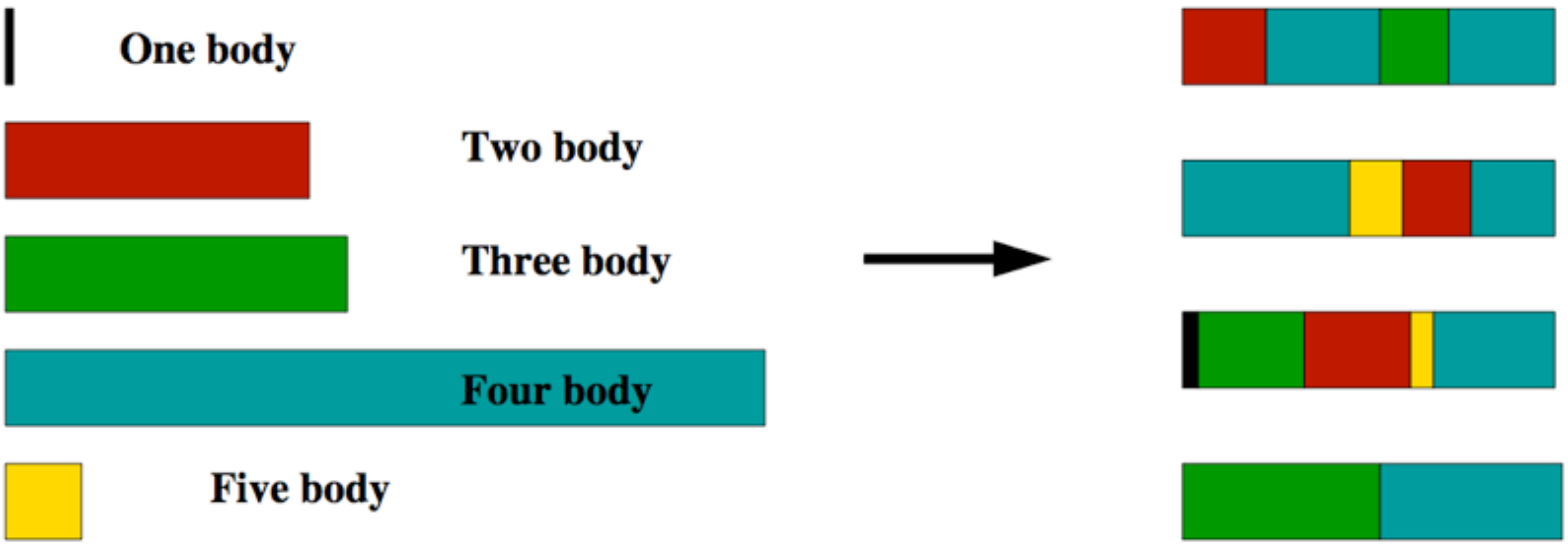


Emmanuel Chang
SciDAC-3 Postdoc

- Transitioning from sequential to integrated production
- Includes GPUs for propagators
- Still need to reduce disk footprint - being done



Workflow (2)

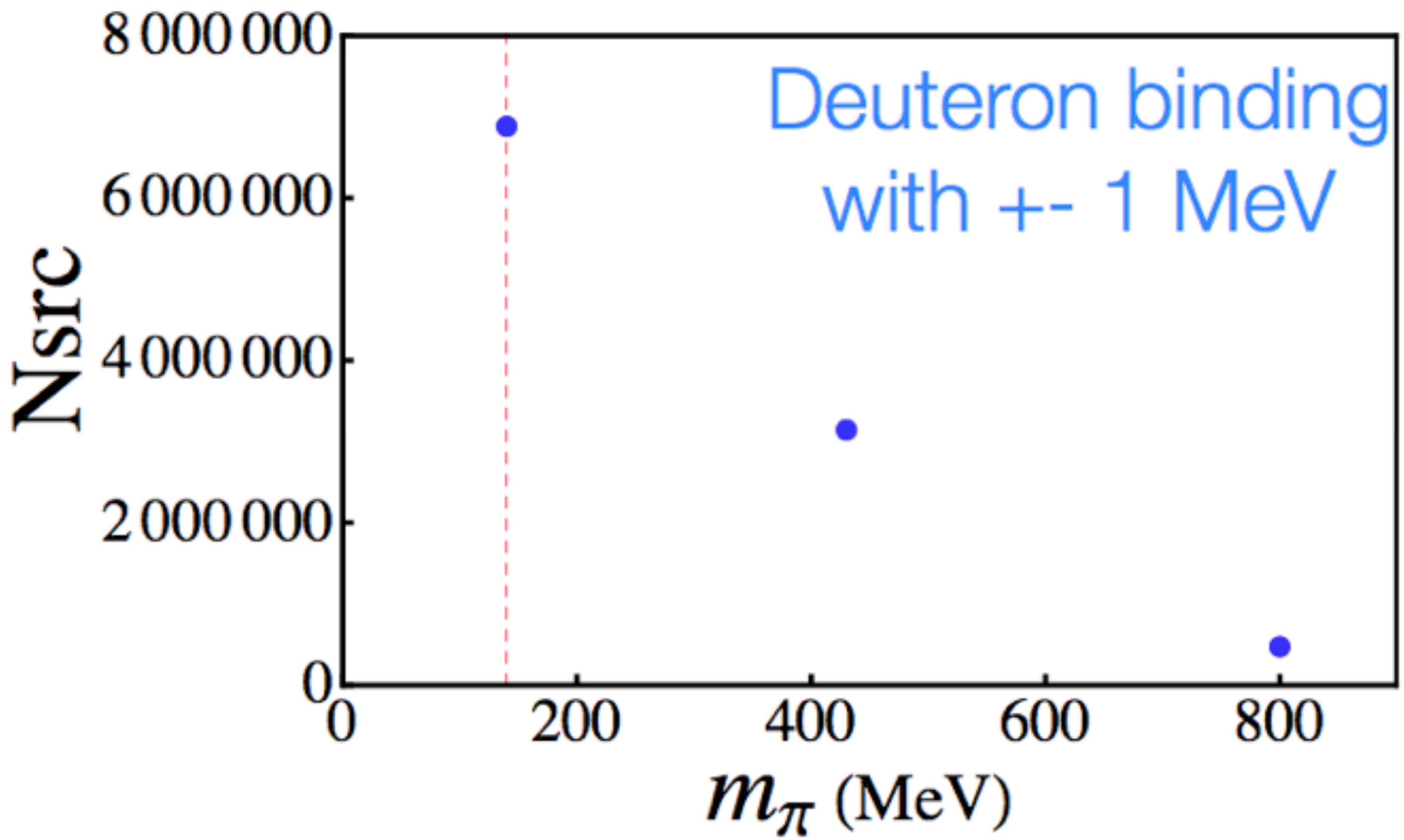


Seperate dependent jobs

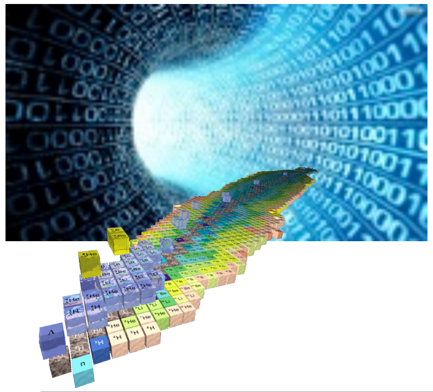
Independent streams of calculation running on cpu cores of a single node after balancing workload

Emmanuel Chang
SciDAC-3 Postdoc

Data Projections



- Physics ``Noise" in nuclear correlation functions
  - variance dictated by pion mass : lighter = noisier
- Remains a petascale problem, as estimated in 2005, 2009, 2011



Data Projections (2)

2012-2014 production

24^3x64, 32^3x64, 48^3x96 lattices , ~ 10^4
500K, 200K, 130K sets

USQCD : 41 M CPU
and 220K GPU

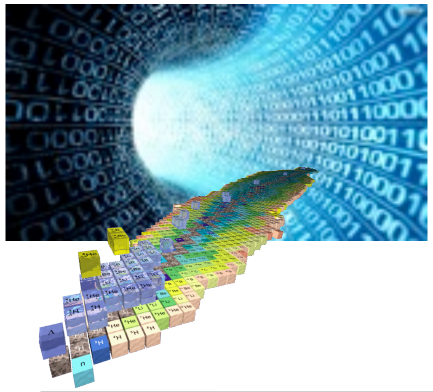
NERSC : 30 M
XSEDE : 20 M

- Checkpointing
  - implicit in workflow
  - manuel restart at present

e.g., 32^3x64

2 props/set

cfg : 1.7 GB
2 prop : 13 GB
2 blocks : 4.4 GB
correlators : 4.2 MB
Saved ~ 17 TB + 1.5 TB
<I/O> ~ 0.14 GB/s



Data Projections (3)

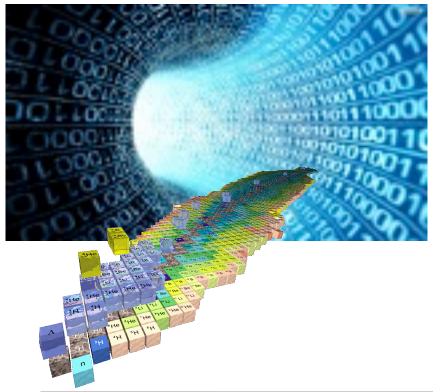
2014-2017 production

64^3x128 lattices , ~ 5 10^3
6M sets

cfg : 27 GB
2 prop : 208 GB
2 blocks : 8.8 GB
correlators : 8.4 MB
Save ~ 135 TB + 50 TB
<I/O> ~ 43 GB/s

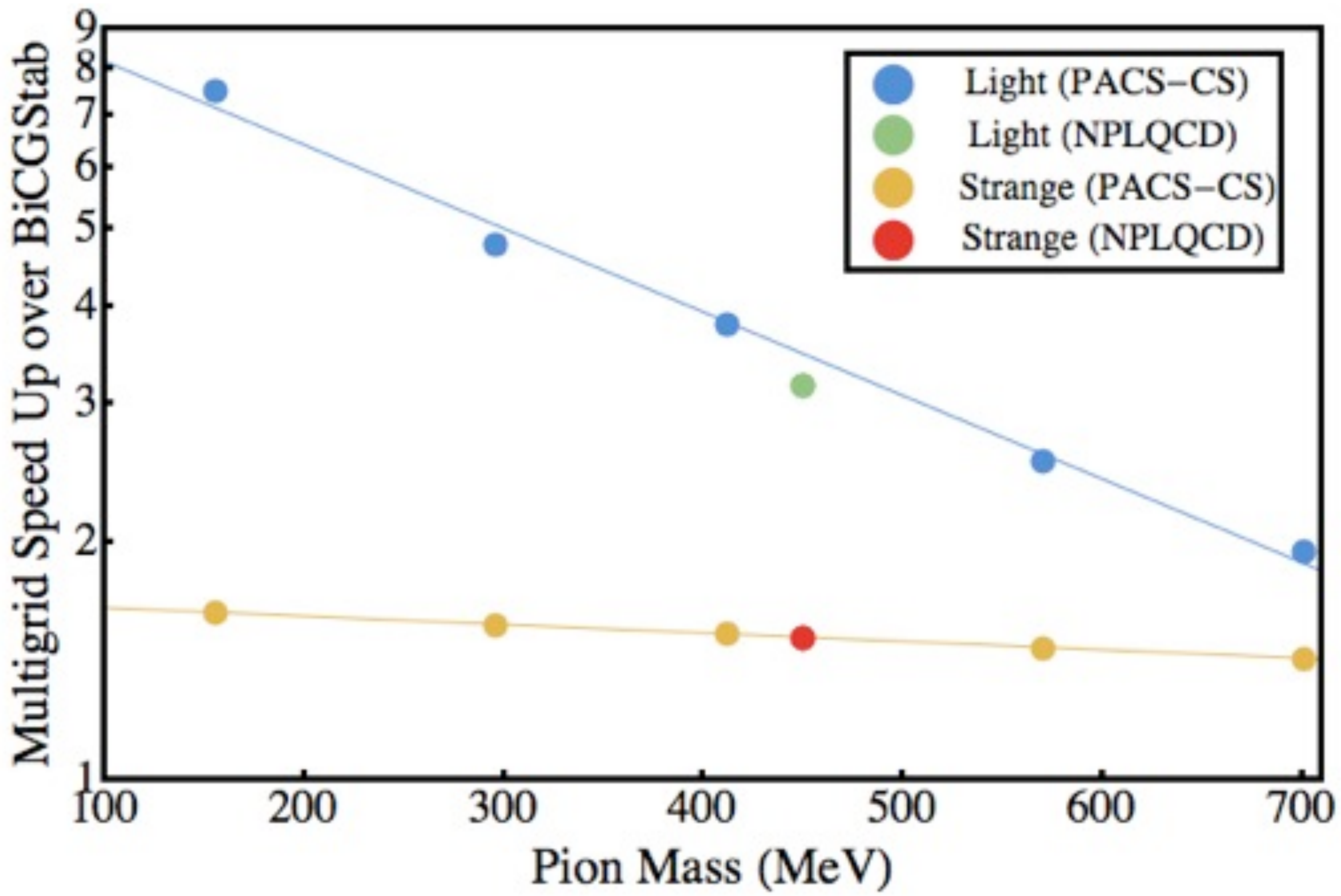
96^3x192 lattices , ~ 5 10^3
6M sets

cfg : 137 GB
2 prop : 1 TB
2 blocks : 13.2 GB
correlators : 12.6 MB
Save ~ 685 TB + 76 TB
writing everything = <I/O> ~ 195 GB/s



Compute

NERSC is ~50% of Nuclear Forces measurement resources

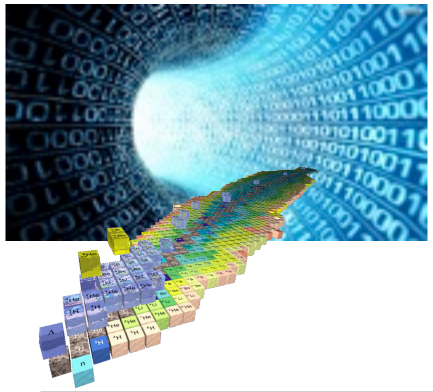


Current NERSC

>16K cores
36 hr run times
80 runs/yr
chroma, usqcd stack, apprec

86 TB reads and 2 TB out
64 GB/node and 50TB global

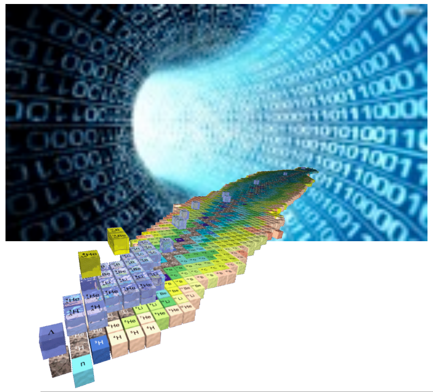
200 TB storage



Compute (2)

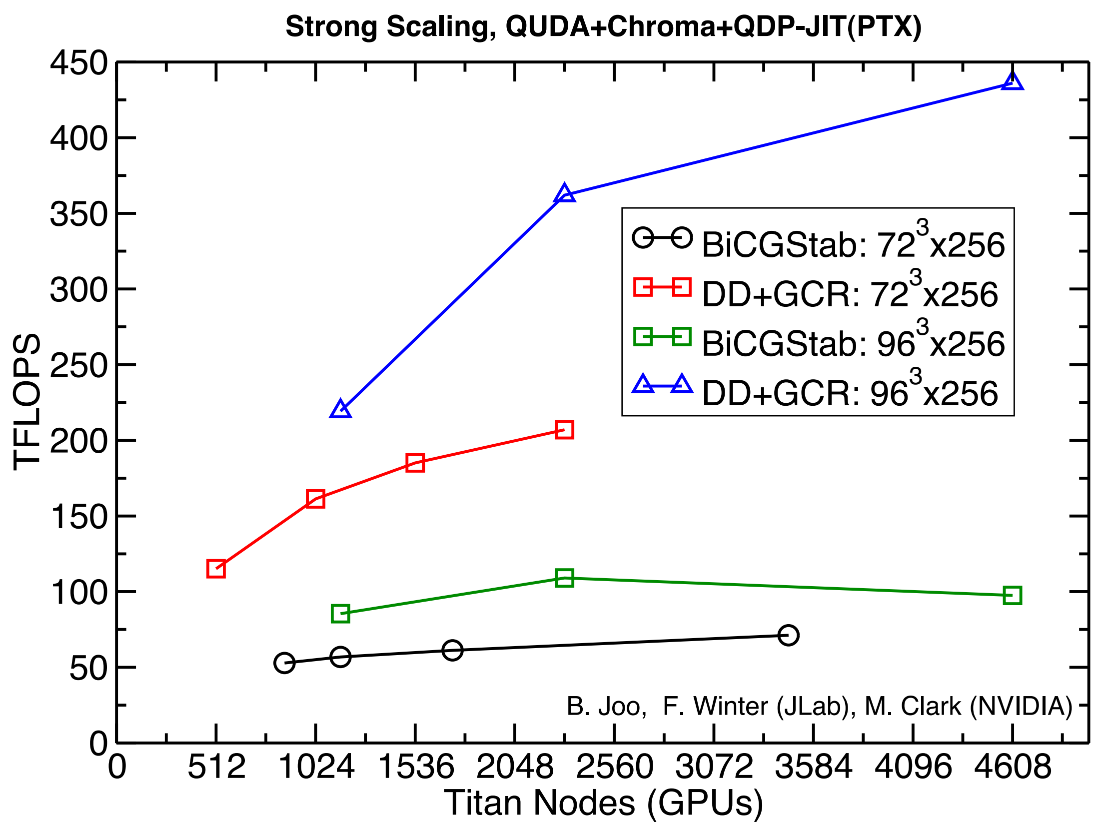
- The highlighted production in the USQCD plan requires 2.8 Bn core-hrs before 2017
  - propagators
  - blocks
  - contractions

- requires ~ 900M core-hrs/year
  - partial co-production with other cold projects
  - < 500 K cores, wallclock limited, as many as needed
  - I/O will be integrated database(s), SQL, hdf5



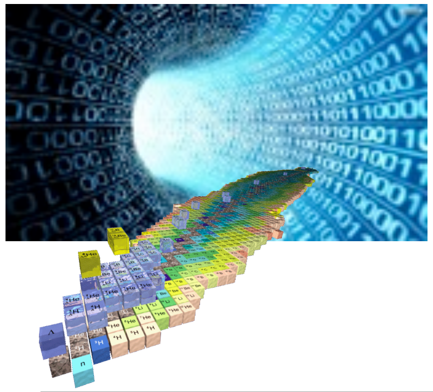
Compute (3)

- Chroma exploits GPU
  - development is ongoing
  - no openCL
- OpenMP in chroma
  - will use soon
- Porting to MIC
  - not yet, will happen



JLab Group
see Robert Edwards presentation

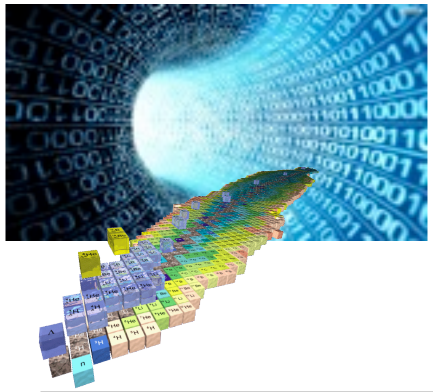
- USQCD/JLab spearheading porting (project non-specific)
  - SciDAC-3



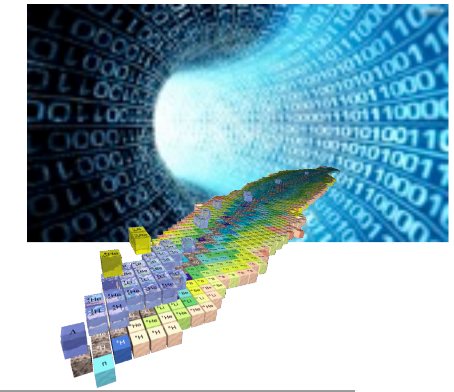
Compute (4)
Things to do ?

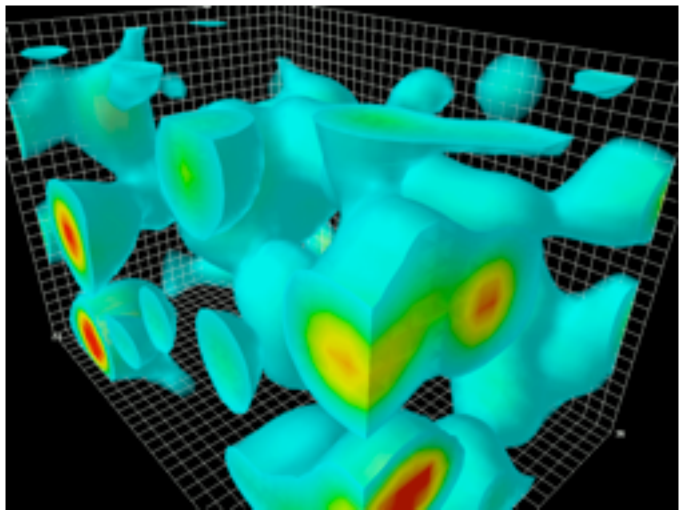
- NERSC
  - People on-site [university] to help port

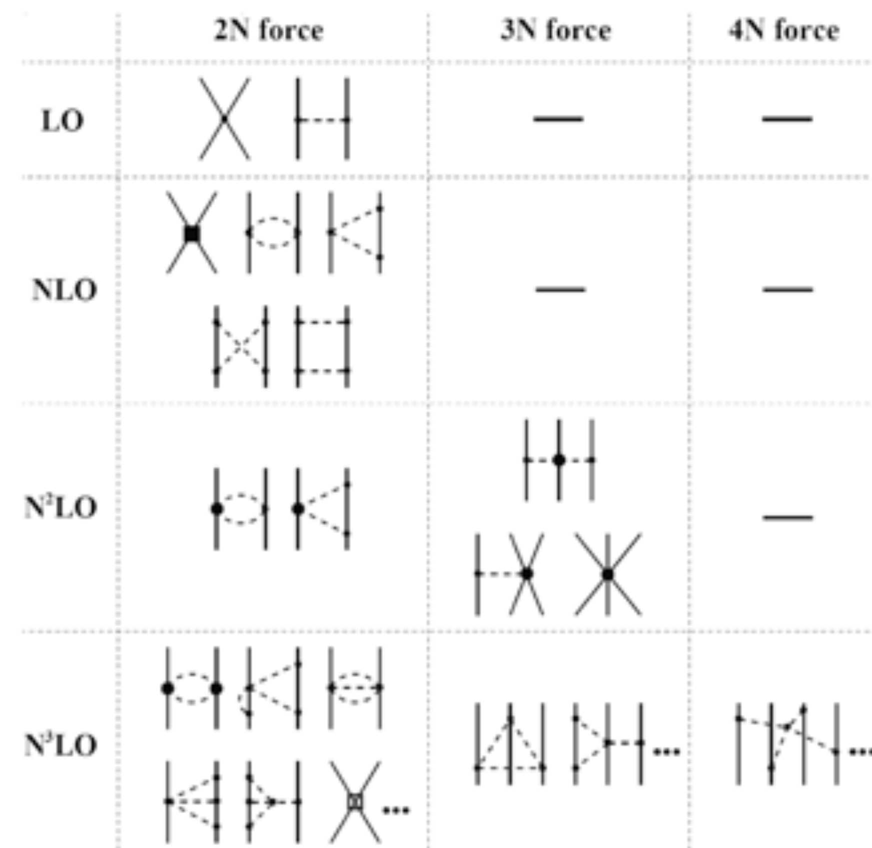
- DOE+ASCR
  - Local development clusters
  - People on-site [university] to help port
  - Full SciDAC-3 support, more postdocs and students



Closing Remarks







Lattice QCD, combined with chiral EFT and nuclear many-body techniques, will provide first principles predictive capabilities for Nuclear Physics

Continuing and increasing large scale NERSC resources are critical to refining nuclear forces

THE END